LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022246.D
Acq On : 27 May 2021 20:35
Operator : JC/MD
Sample : M2520-02 40X
Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-02-2021-05-24

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Title : SW846 8260

Signal : TIC: VX022246.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.397	696	707	722	rVB	50679	142631	4.81%	1.256%
2	5.562	722	734	747	rBV2	79214	222604	7.51%	1.961%
3	5.964	791	800	817	rVB3	64195	165118	5.57%	1.455%
4	6.769	921	932	950	rBV	142920	335999	11.34%	2.960%
5	8.653	1234	1241	1249	rBV	316395	478488	16.15%	4.215%
6	10.055	1465	1471	1482	rBV	298900	401846	13.56%	3.540%
7	10.195	1489	1494	1504	rVB	133799	173835	5.87%	1.531%
8	10.963	1616	1620	1628	rBV	26018	32858	1.11%	0.289%
9	11.085	1634	1640	1648	rBV	230322	290301	9.80%	2.557%
10	11.616	1722	1727	1734	rBV	36000	45569	1.54%	0.401%
11	11.756	1741	1750	1755	rBV	123140	151955	5.13%	1.339%
12	12.024	1789	1794	1800	rVB	305919	380846	12.86%	3.355%
13	12.091	1800	1805	1809	rBV	52937	63630	2.15%	0.561%
14	12.244	1825	1830	1838	rBV	597216	741984	25.05%	6.536%
15	12.317	1838	1842	1848	rVV3	25374	38466	1.30%	0.339%
16	12.616	1886	1891	1895	rBV	62313	75281	2.54%	0.663%
17	12.701	1901	1905	1911	rBV	32597	47916	1.62%	0.422%
18	12.963	1945	1948	1954	rBV	32895	42784	1.44%	0.377%
19	13.170	1978	1982	1987	rBV	80908	94928	3.20%	0.836%
20	13.292	1998	2002	2007	rBV2	51294	67160	2.27%	0.592%
21	13.347	2007	2011	2016	rVV	106813	129939	4.39%	1.145%
22	13.426	2019	2024	2029	rVB	190721	244405	8.25%	2.153%
23	13.548	2040	2044	2047	rBV	24708	31622	1.07%	0.279%
24	13.780	2074	2082	2090	rBV	2408494	2962526	100.00%	26.097%
25	13.871	2090	2097	2103	rVV	72800	102114	3.45%	0.900%
26	14.225	2150	2155	2158	rBV	39601	56789	1.92%	0.500%
27	14.323	2164	2171	2177	rBV	38617	66841	2.26%	0.589%
28	14.603	2211	2217	2219	rVV	28908	39836	1.34%	0.351%
29	14.640	2219	2223	2233	rVB2	130535	187218	6.32%	1.649%
30	14.780	2241	2246	2257	rVB	955370	1270765	42.89%	11.194%
31	15.206	2308	2316	2322	rBV	107627	150759	5.09%	1.328%
32	15.377	2333	2344	2347	rBV	82020	144053	4.86%	1.269%
33	15.414	2347	2350	2354	rVB	40089	53907	1.82%	0.475%
34	15.481	2354	2361	2366	rBV	224933	365166	12.33%	3.217%
35	15.615	2372	2383	2387	rBV	266816	460589	15.55%	4.057%
36	15.652	2387	2389	2396	rVB	91938	126293	4.26%	1.113%

LSC Area Percent Report

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Operator : JC/MD
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Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-02-2021-05-24

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Title : SW846 8260

37	15.841	2410	2420	2432	rVB3	81714	234849	7.93%	2.069%
38	15.993	2438	2445	2454	rVB2	54660	95971	3.24%	0.845%
39	16.090	2455	2461	2468	rBV	34724	56063	1.89%	0.494%
40	16.334	2492	2501	2510	rBV2	203884	446552	15.07%	3.934%
41	16.566	2530	2539	2541	rBV5	14413	32101	1.08%	0.283%
42	16.603	2541	2545	2550	rVV2	22884	45594	1.54%	0.402%
43	16.664	2550	2555	2566	rVB3	21308	53638	1.81%	0.473%

Sum of corrected areas: 11351789

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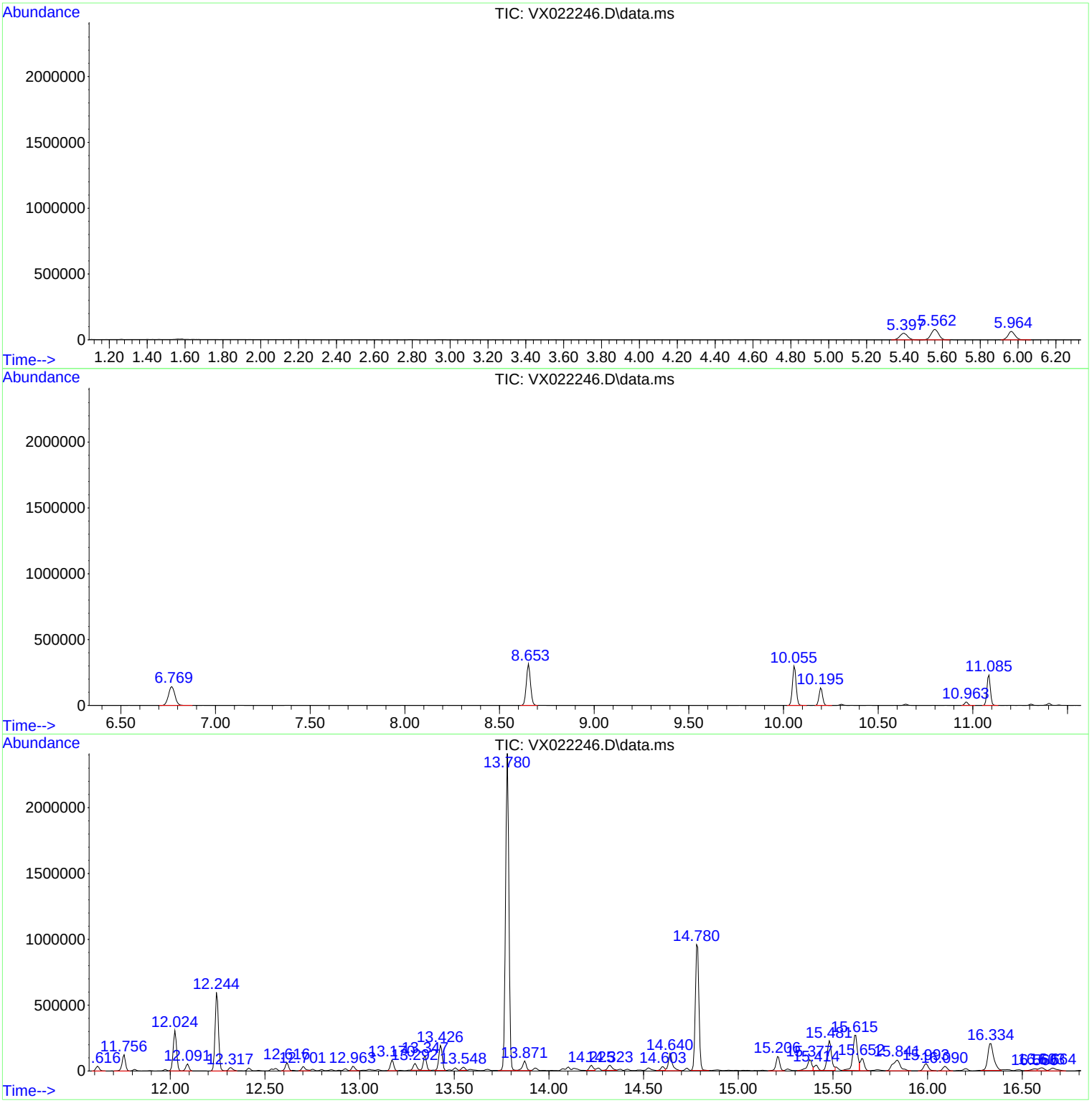
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022246.D
Acq On : 27 May 2021 20:35
Operator : JC/MD
Sample : M2520-02 40X
Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

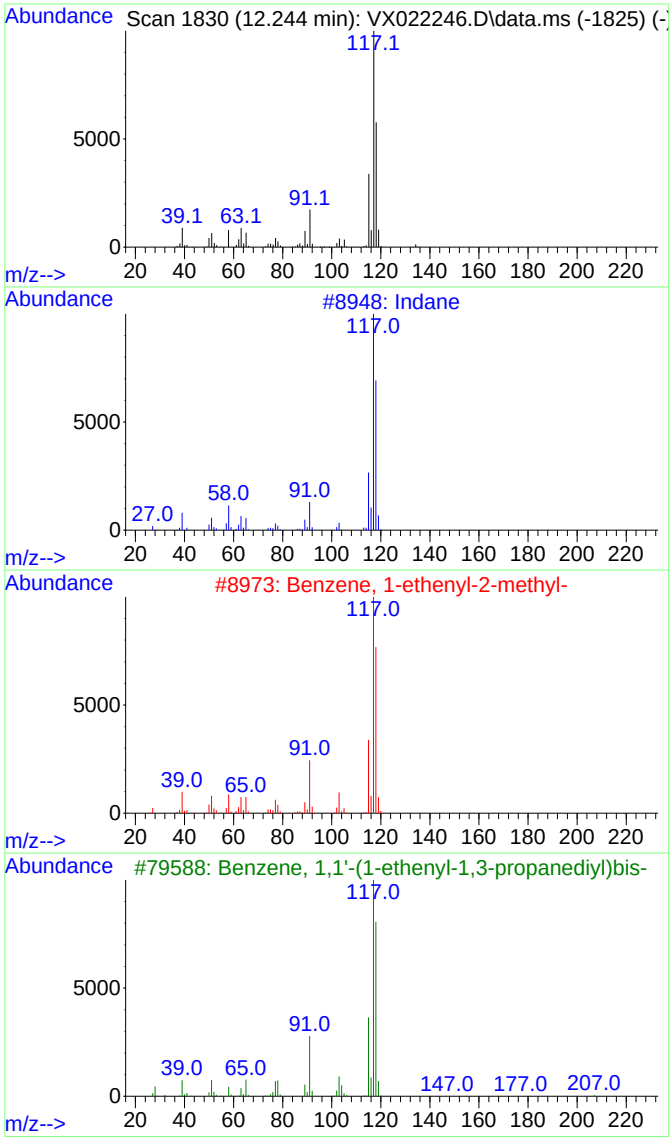
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

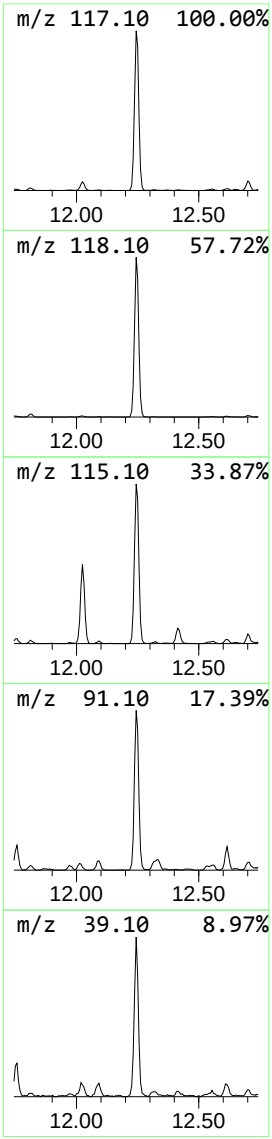
****

Peak Number 1 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	97.41 ug/l	741984	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
3	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	78
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	74





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Data File : VX022246.D
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Operator : JC/MD
Sample : M2520-02 40X
Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

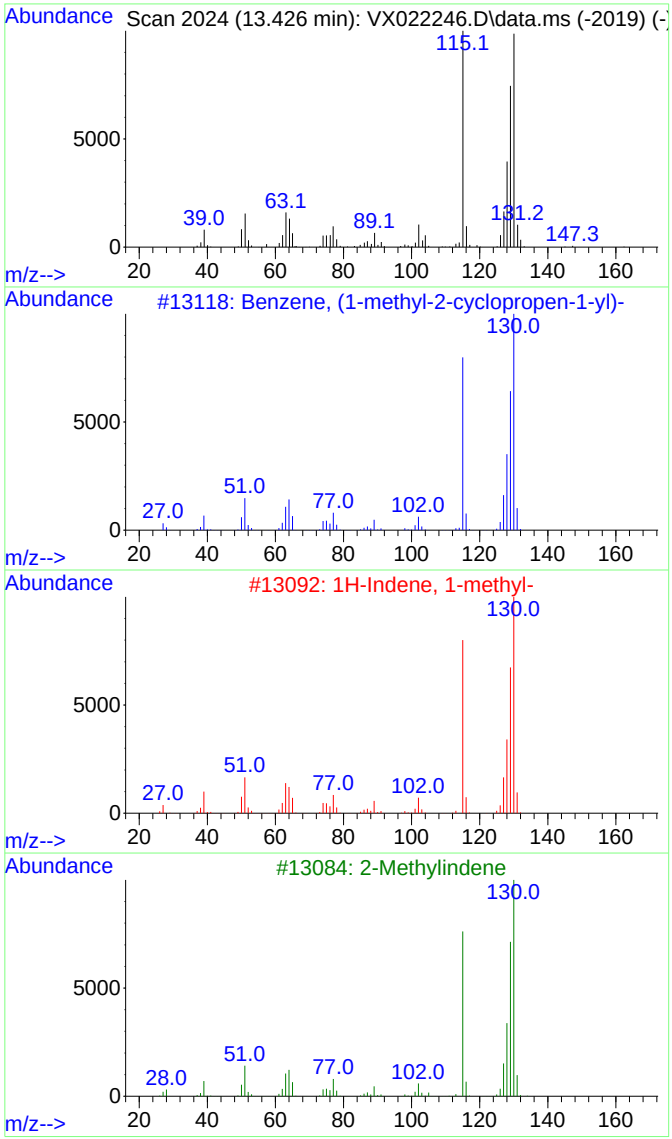
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

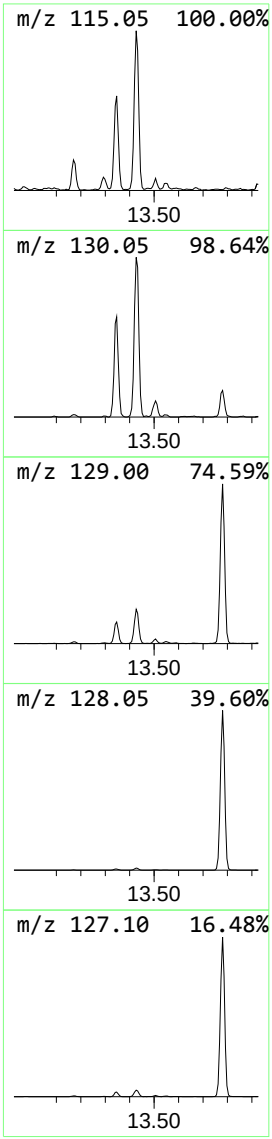
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, (1-methyl-2-cyclop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	32.09 ug/l	244405	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3	2-Methylindene	130	C10H10	002177-47-1	96
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022246.D
Acq On : 27 May 2021 20:35
Operator : JC/MD
Sample : M2520-02 40X
Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

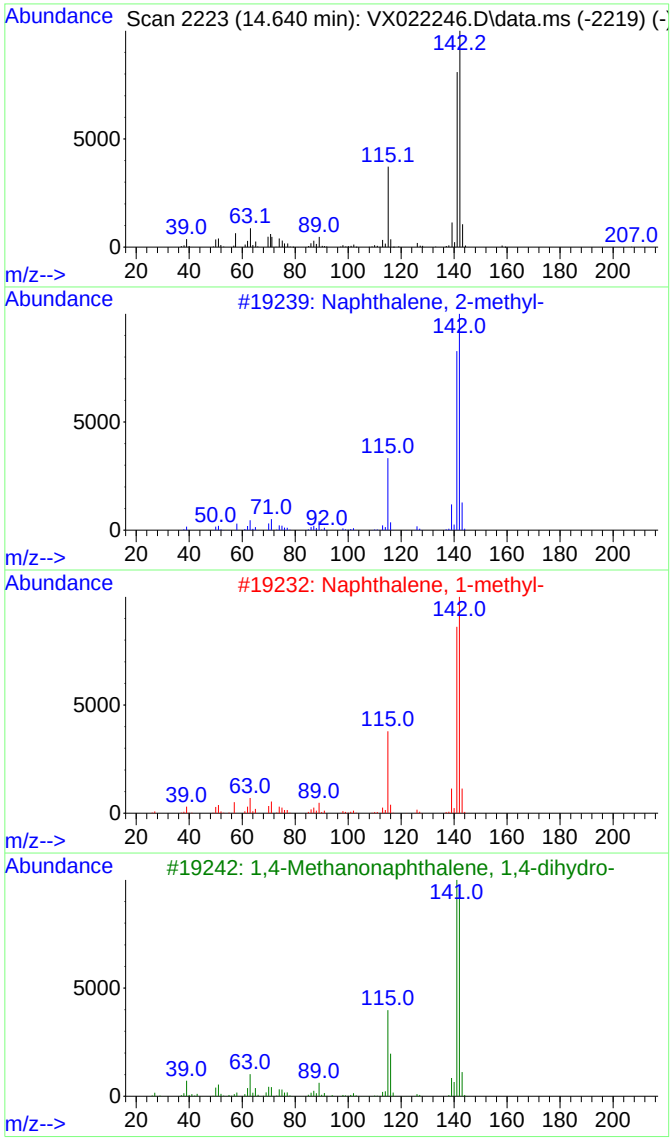
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

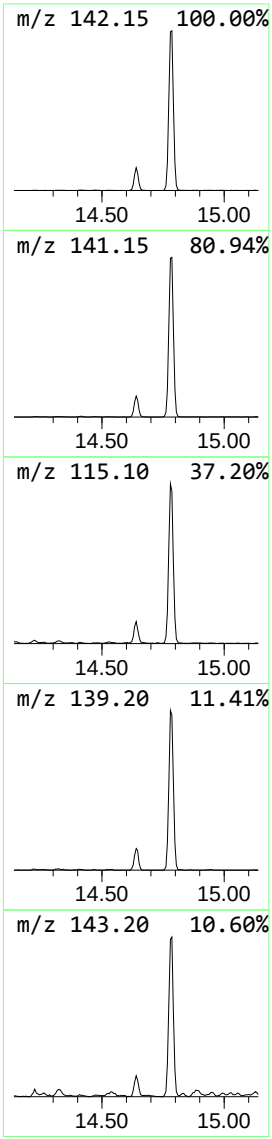
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	24.58 ug/l	187218	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72
5	Benzocycloheptatriene	142	C11H10	000264-09-5	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022246.D
Acq On : 27 May 2021 20:35
Operator : JC/MD
Sample : M2520-02 40X
Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

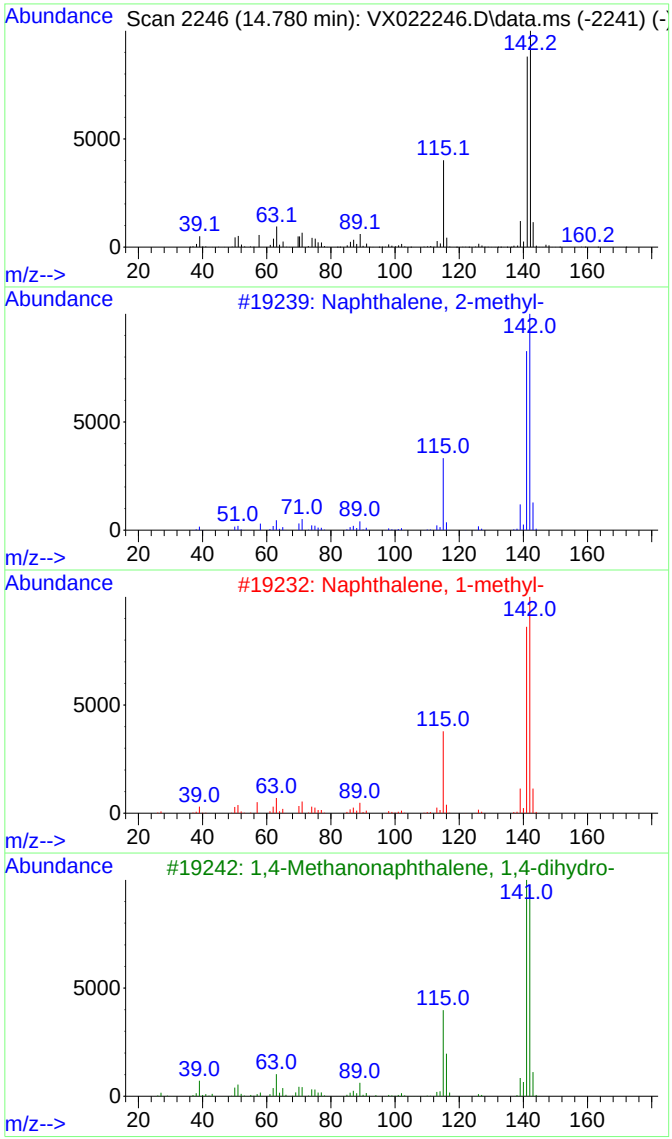
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

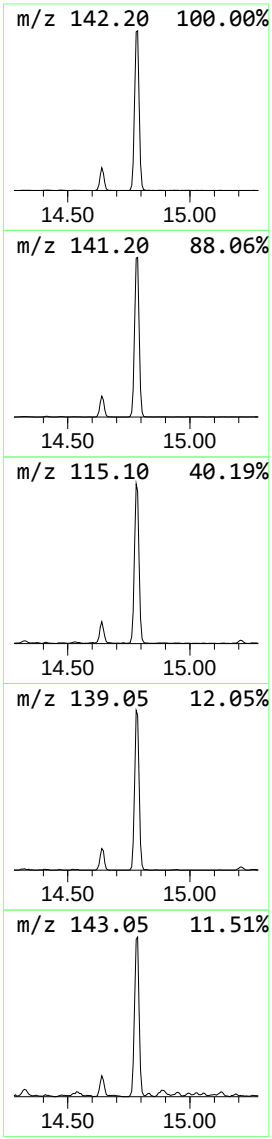
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1,4-Methanonaphthalene, 1,4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	166.83 ug/l	1270770	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5	Benzocycloheptatriene	142	C11H10	000264-09-5	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
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Acq On : 27 May 2021 20:35
Operator : JC/MD
Sample : M2520-02 40X
Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
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TIC Library : C:\DATABASE\NIST11.L
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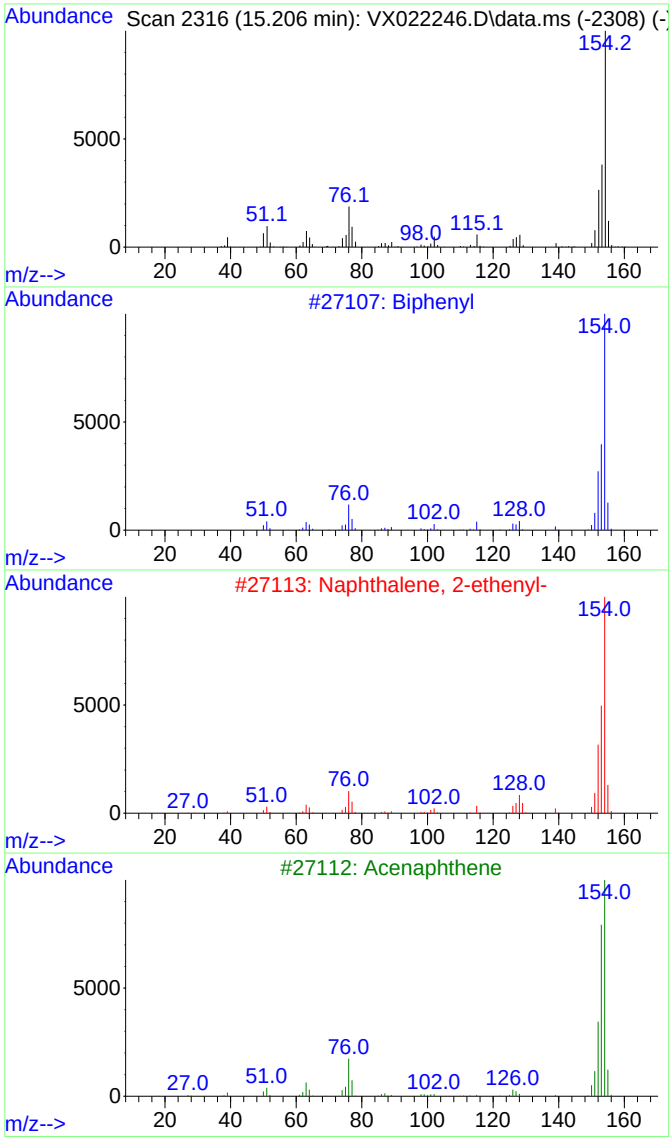
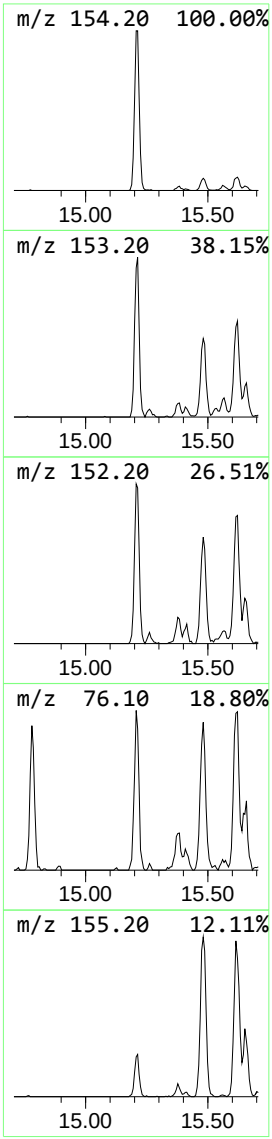
****

Peak Number 5 Biphenyl Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	19.79 ug/l	150759	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Biphenyl	154	C12H10	000092-52-4	95
2	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	91
3	Acenaphthene	154	C12H10	000083-32-9	60
4	2-Quinolinecarbonitrile	154	C10H6N2	001436-43-7	47
5	1-Isoquinolinecarbonitrile	154	C10H6N2	001198-30-7	38





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Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

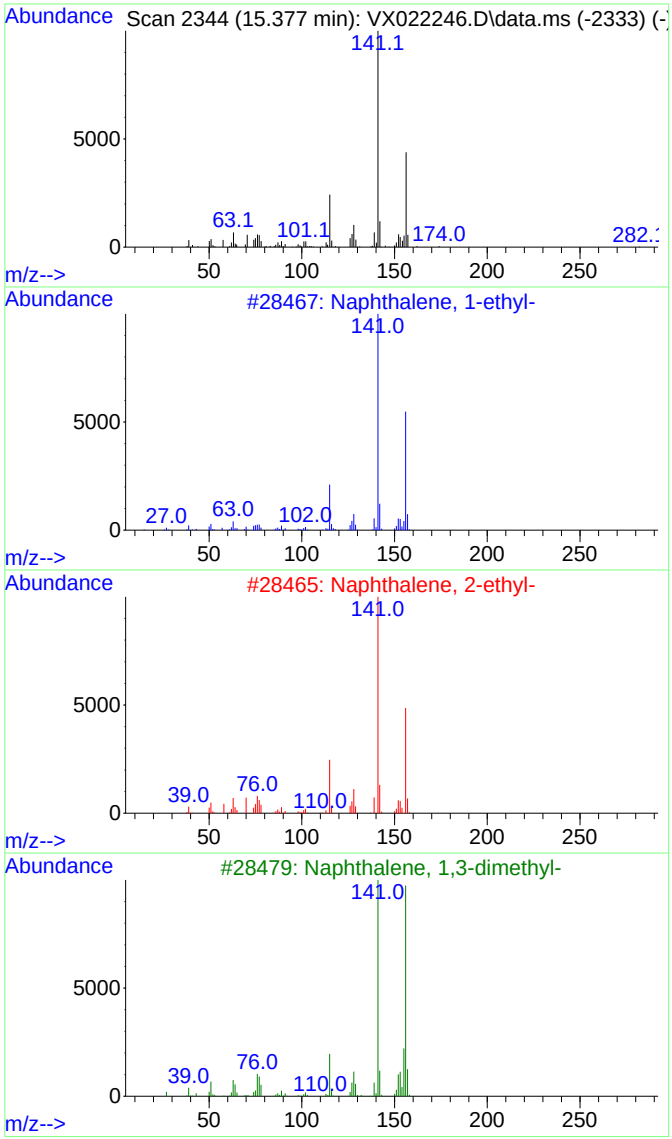
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

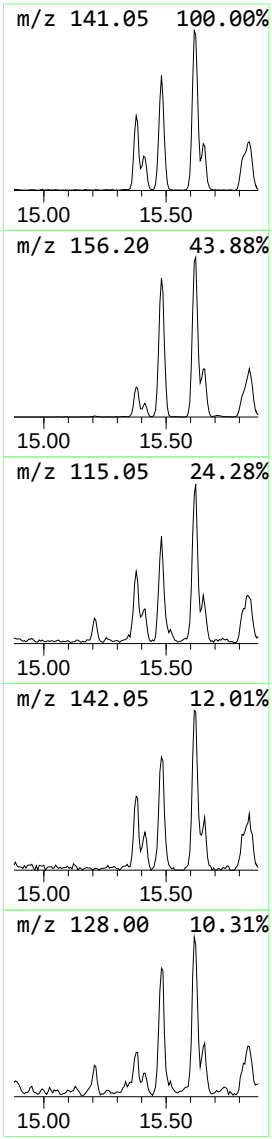
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 1-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.377	18.91 ug/l	144053	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	95
2	Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	95
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	80
4	2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	59
5	Butethal	212	C10H16N2O3	000077-28-1	59





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Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

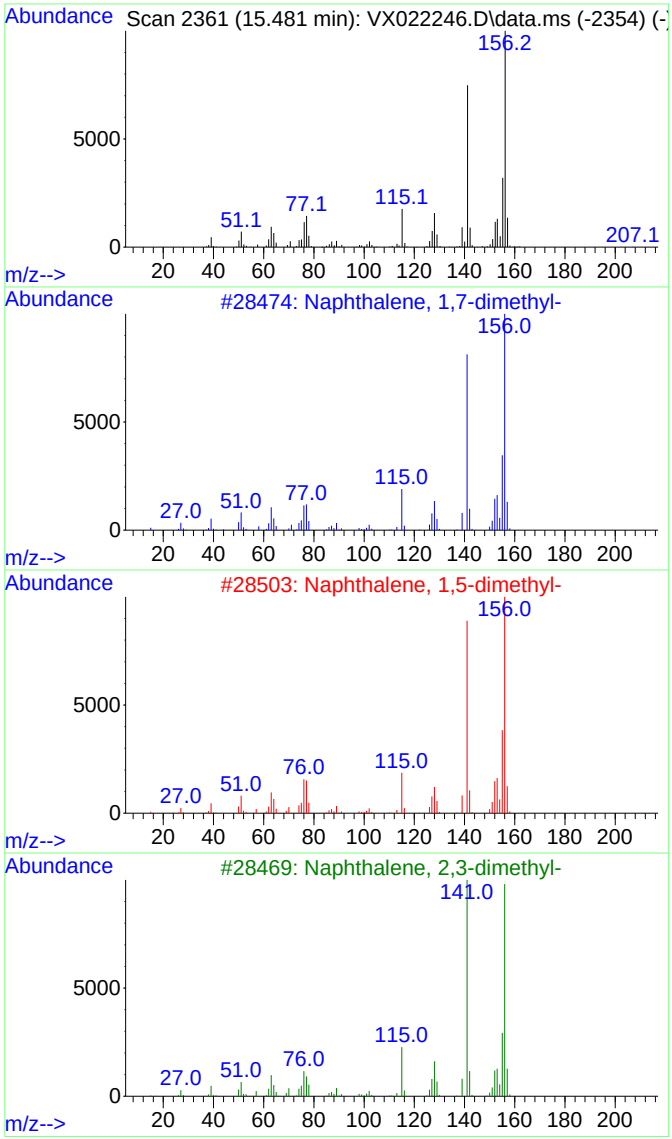
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

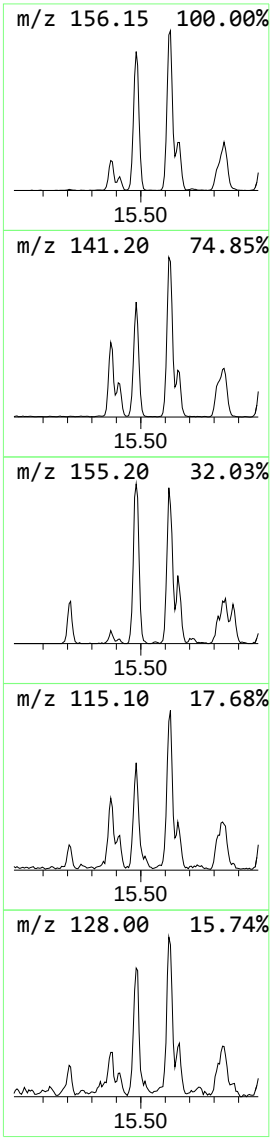
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	47.94 ug/l	365166	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	98
2	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	98
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022246.D
Acq On : 27 May 2021 20:35
Operator : JC/MD
Sample : M2520-02 40X
Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

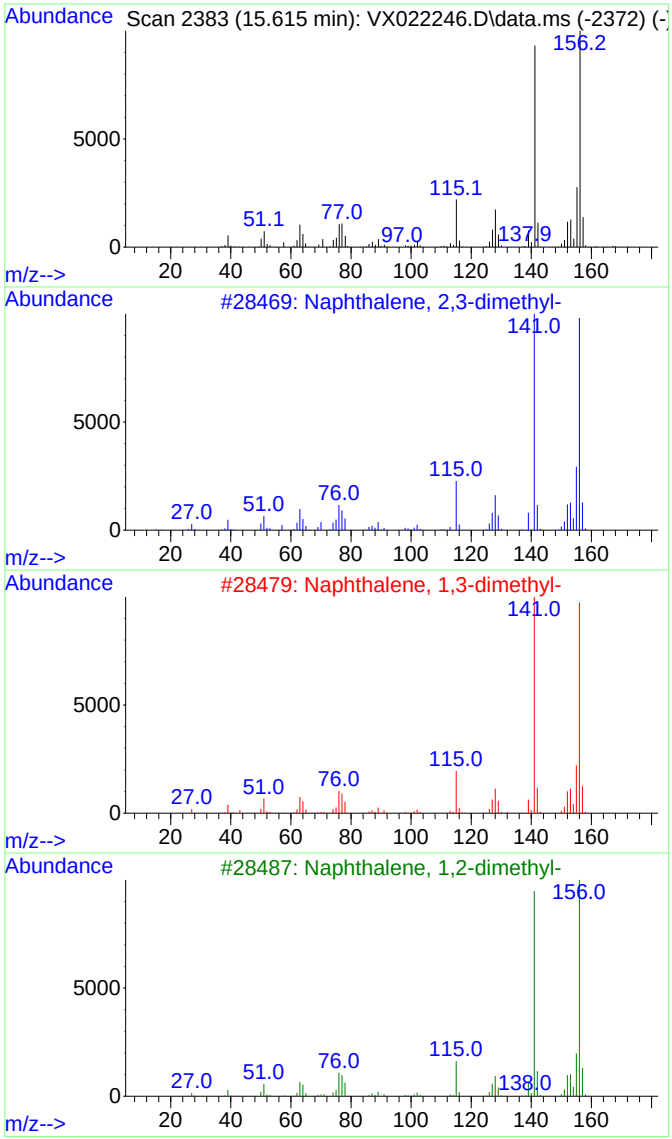
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

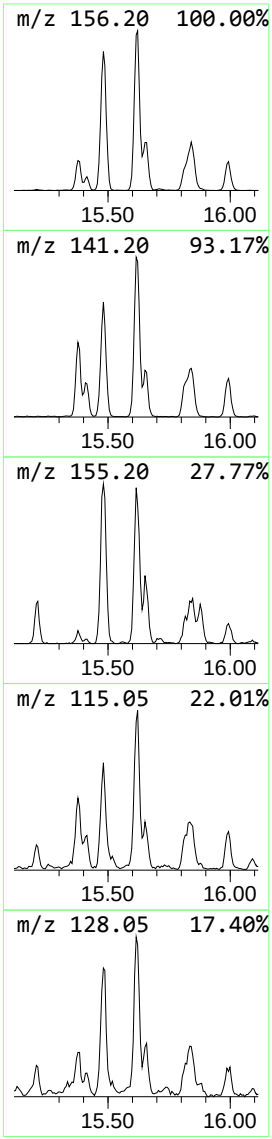
****

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	60.47 ug/l	460589	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022246.D
Acq On : 27 May 2021 20:35
Operator : JC/MD
Sample : M2520-02 40X
Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

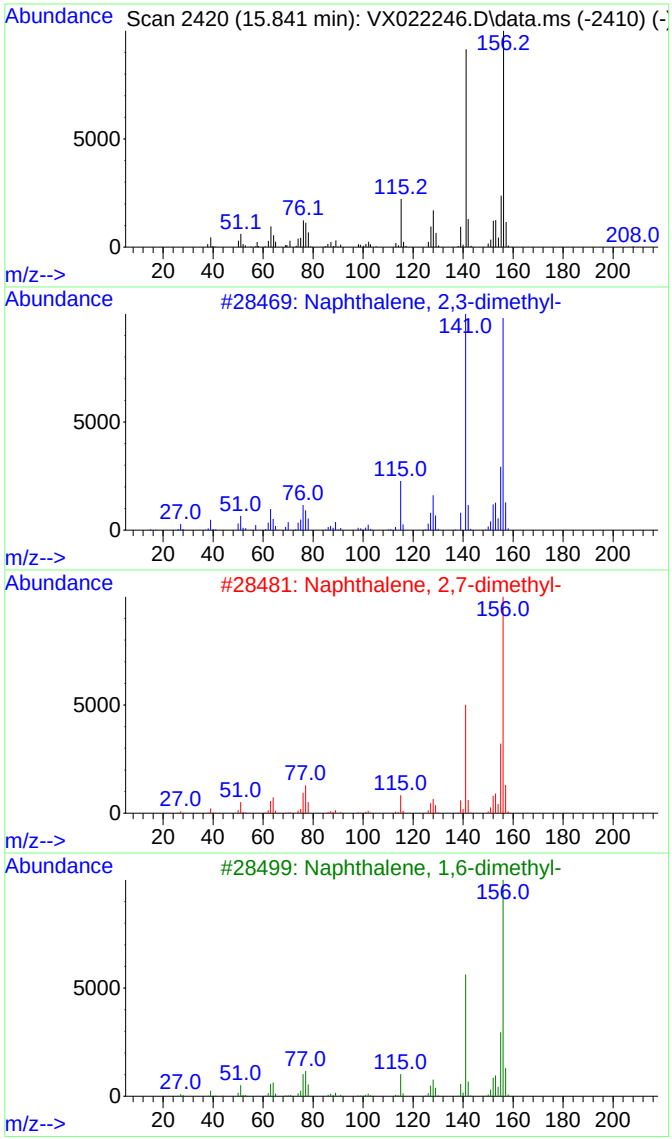
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

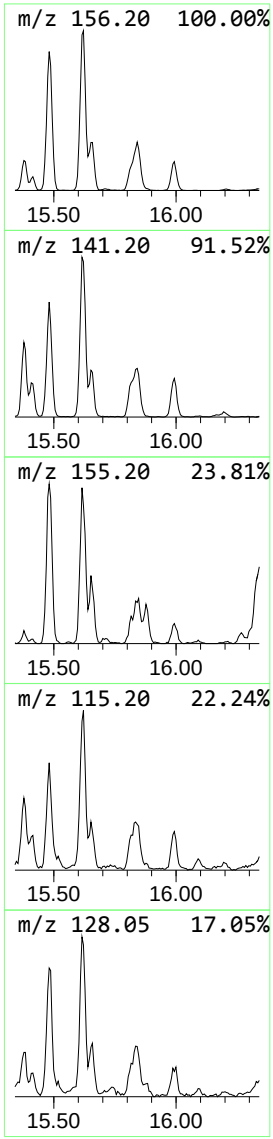
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 2,7-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	30.83 ug/l	234849	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022246.D
Acq On : 27 May 2021 20:35
Operator : JC/MD
Sample : M2520-02 40X
Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

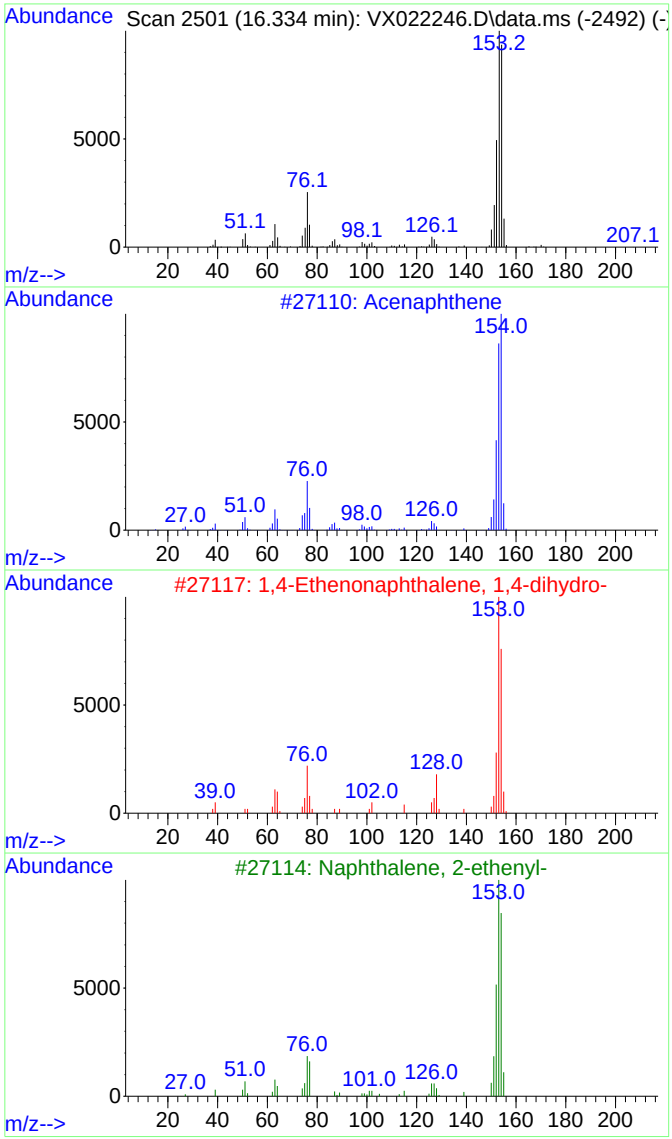
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

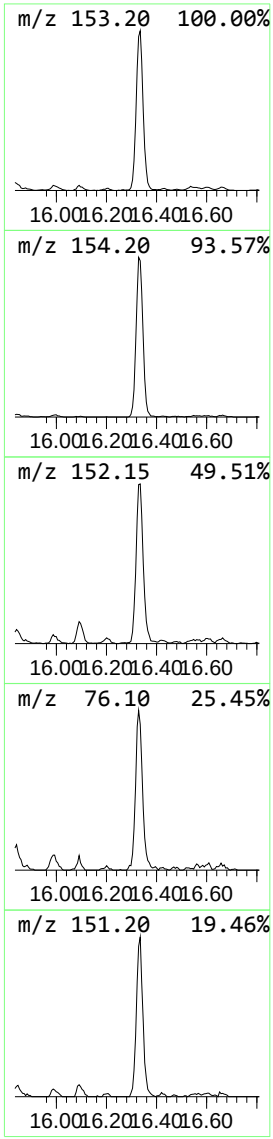
****

Peak Number 10 Acenaphthene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.334	58.63 ug/l	446552	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	95
2	1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	64
3	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	62
4	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5	Biphenyl	154	C12H10	000092-52-4	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022246.D
Acq On : 27 May 2021 20:35
Operator : JC/MD
Sample : M2520-02 40X
Misc : 15.039g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-02-2021-05-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Indane	12.244	97.4	ug/l	741984	4	12.024	380846	50.0
Benzene, (1-met...	13.426	32.1	ug/l	244405	4	12.024	380846	50.0
Naphthalene, 1-...	14.640	24.6	ug/l	187218	4	12.024	380846	50.0
1,4-Methanonaph...	14.780	166.8	ug/l	1270770	4	12.024	380846	50.0
Biphenyl	15.207	19.8	ug/l	150759	4	12.024	380846	50.0
Naphthalene, 1-...	15.377	18.9	ug/l	144053	4	12.024	380846	50.0
Naphthalene, 1,...	15.481	47.9	ug/l	365166	4	12.024	380846	50.0
Naphthalene, 2,...	15.615	60.5	ug/l	460589	4	12.024	380846	50.0
Naphthalene, 2,...	15.841	30.8	ug/l	234849	4	12.024	380846	50.0
Acenaphthene	16.334	58.6	ug/l	446552	4	12.024	380846	50.0